

Spectral functions and correlations in a bosonic Josephson junction

David López Núñez

Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.

Abstract: We analyse the properties of an ultracold atomic cloud trapped in an external double-well potential with the Bose-Hubbard approximation. We characterize the many-body properties of the system through the study of the single-particle spectral functions, identifying the different regimes that the system exhibits for all the possible parameters in this approach.

I. INTRODUCTION

The realization of the Bose-Einstein condensation (BEC) made a major development in quantum physics since it provided a useful set up to experiment new phenomena in many fields observing quantum physics at a macroscopic level. In recognition of its importance and directly related to its first realization, two Nobel prizes have been awarded.

Bose-Einstein condensation is a phenomenon that can occur in systems made of particles which obey the Bose-Einstein statistics. At zero temperature, $T = 0$, or sufficiently low temperature, a large fraction of bosons populate the same single-particle (sp) state, resulting in a macroscopically occupied quantum state. Although it was predicted by Einstein for non-interacting systems, it has been seen that it occurs also in strongly interacting systems, such as liquid ^4He . The interactions do not destroy the condensate, they only remove a few particles from the condensate.

In this work we consider ultracold and dilute bosons confined in a one-dimensional double well, which has been termed bosonic Josephson junction [1]. The physics of bosons trapped in a double-well potential has attracted a lot of attention and it has been recently achieved experimentally in Prof. Oberthaler's group in Heidelberg [1–3] and in the group of Prof. Schmiedmayer [4] in Vienna.

The double well can be realized by confining the bosons with a superposition of a strong isotropic harmonic confinement in the transverse plane and a symmetric double-well potential in the axial direction. The interaction between the bosons is due to a short-range contact potential. This interaction can be either repulsive or attractive, resulting in different behaviours. Experimentally, only the first kind of interaction has been already achieved.

Depending on the type of interaction, the ground state of the system shows different properties. For the repulsive case, by increasing the interaction, the system undergoes a crossover from a coherent state to a pure Fock state, with half of the particles in each side. While in the attractive case, with a small symmetry-breaking bias, the system goes from the coherent regime to a completely asymmetric Fock state, where all the particles are in one side, passing through a cat-like state.

The double-well physics can be successfully characterized by a model of two sp-states, one located in each well, since we can assume that there is only one relevant sp-state in each well.

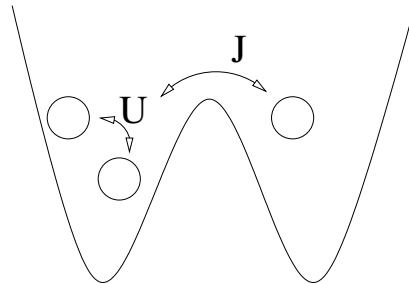


FIG. 1. Schematic figure of the system consisting in a double-well potential with interaction between particles, U , and tunnelling, J .

II. THEORETICAL MODEL

This system can be studied with a simple approach, the two-mode Bose-Hubbard Hamiltonian for N atoms,

$$\hat{H} = \frac{U}{2} [\hat{n}_L(\hat{n}_L - 1) + \hat{n}_R(\hat{n}_R - 1)] - J (\hat{a}_R^\dagger \hat{a}_L + \hat{a}_L^\dagger \hat{a}_R) - \epsilon (\hat{n}_L - \hat{n}_R) \quad (1)$$

where $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$, $\hat{a}_L^\dagger |n_L, n_R\rangle = \sqrt{n_L + 1} |n_L + 1, n_R\rangle$, $\hat{a}_L |n_L, n_R\rangle = \sqrt{n_L} |n_L - 1, n_R\rangle$, $[\hat{a}_i^\dagger, \hat{a}_j] = \delta_{ij}$ and $[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$, $i, j = L, R$. $L(R)$ represents the left (right) side of the well.

The first term of the Hamiltonian, $\hat{V}_1 = \frac{U}{2} [\hat{n}_L(\hat{n}_L - 1) + \hat{n}_R(\hat{n}_R - 1)]$, is the one caused by the atomic interaction between atoms located in the same well. Our sign convention is such that $U > 0$ ($U < 0$) corresponds to a repulsive (attractive) interaction. The second term is $\hat{V}_2 = -J (\hat{a}_R^\dagger \hat{a}_L + \hat{a}_L^\dagger \hat{a}_R)$, which describes the tunnelling effect, being J the hopping amplitude between the two wells (taken positive). Finally, a small bias is introduced, $0 < \epsilon \ll J$ to break the left-right symmetry when the system has to choose between the two wells (in this case, as ϵ is taken positive, the left side will be chosen).

In recent works [5], another potential has been added, $\hat{V}_3 = W \hat{n}_L \hat{n}_R$. This potential introduces an interaction caused by a dipole force between particles sitting at different wells. The addition of this potential allows to explore the same physical behaviours, such as the macroscopic cat-state, without the necessity of an attractive

interaction, $U < 0$, which is difficult to achieve experimentally.

To obtain the eigenvectors and eigenvalues of the Hamiltonian, we perform an exact diagonalization in the $N + 1$ dimensional space spanned by the Fock basis, $(|N, 0\rangle, |N - 1, 1\rangle \dots |0, N\rangle)$. To simplify the notation, we will define $|n_L, n_R\rangle \equiv |n_L\rangle$, but we have to remember how many particles there are in the system. In the second quantization language, $|n_L\rangle = 1/\sqrt{n_L!(N - n_L)!}(\hat{a}_L^\dagger)^{n_L}(\hat{a}_R^\dagger)^{N - n_L}|vac\rangle$. Hence a general state will be written

$$|\Psi_m^N\rangle = \sum_{i=0}^N C_{i,N}^m |i\rangle. \quad (2)$$

The subscript on Ψ (superscript in C) means that we have the ground state, if $m = 0$, or an excited state, if $m > 0$, and the superscript N (subscript in C) indicates the number of particles in the system.

As shown in previous papers [6, 7], the properties of the system are governed by the parameter $\Lambda \equiv NU/J$. To tune this parameter, we will always modify, theoretically speaking, the interaction term U .

To characterize the system one uses the one-body density matrix $\hat{\rho}$. For a state $|\phi\rangle$ it is defined as $\hat{\rho}_{ij} = \langle\phi|a_i^\dagger a_j|\phi\rangle$ where $i, j = L, R$, or the basis considered. The eigenvalues and the natural orbits (i.e. eigenvectors) of the one-body density matrix are independent of the chosen basis and it provides a very valuable information of the system. For instance, if there is only one eigenvalue different from zero, the system is fully condensed in the corresponding natural orbit. This is a 2x2 matrix, since there are only two independent sp-states.

In this work we will consider a complementary characterization by studying the single-particle spectral functions (SPSF). First we will define both the hole and the particle SPSF. For the left state $|L\rangle$,

$$S_h(L, L, E) = \sum_n |\langle\Psi_n^{N-1} | \hat{a}_L | \Psi_0^N\rangle|^2 \times \delta(E - (E_0^N - E_n^{N-1})) \quad (3)$$

$$S_p(L, L, E) = \sum_m |\langle\Psi_m^{N+1} | \hat{a}_L^\dagger | \Psi_0^N\rangle|^2 \times \delta(E - (E_m^{N+1} - E_0^N)). \quad (4)$$

These SPSF can be defined for every possible sp-state. For instance, $|R\rangle$, but we will also analyse them for the superposition states $|+\rangle \equiv 1/\sqrt{2}(|L\rangle + |R\rangle)$ and $|-\rangle \equiv 1/\sqrt{2}(|L\rangle - |R\rangle)$. It could be also defined for mixed terms as $S_h(L, R, E)$. Note that the SPSF will have several peaks, located at the excitation energies.

Apart from these strengths, the SPSF contain more physical information. For instance, the occupation of the sp-state i , $n_i = \int_{-\infty}^{\mu^-} dE S_h(i, i, E)$, where $\mu^- \equiv E_0^N - E_0^{N-1}$. They also provide sum tests to prove the accuracy of our results.

The first test is due to the commutation relation between the creation and annihilation Bose operators,

$$\int_{-\infty}^{+\infty} dE [S_p(i, i, E) - S_h(i, i, E)] = \sum_m \langle\Psi_0^N | \hat{a}_i | \Psi_m^{N+1}\rangle \langle\Psi_m^{N+1} | \hat{a}_i^\dagger | \Psi_0^N\rangle - \sum_n \langle\Psi_0^N | \hat{a}_i^\dagger | \Psi_n^{N-1}\rangle \langle\Psi_n^{N-1} | \hat{a}_i | \Psi_0^N\rangle = \langle\Psi_0^N | [\hat{a}_i, \hat{a}_i^\dagger] | \Psi_0^N\rangle = 1 \quad (5)$$

which is valid for every i -state.

The Koltum sum-rule is very useful because it provides the energy of the system. Let's calculate firstly the energy weighed sum-rule for the hole SPSF,

$$I_\alpha = \int_{-\infty}^{\mu^-} dE E S_h(\alpha, \alpha, E) = \sum_m (E_0^N - E_m^{N-1}) \langle\Psi_0^N | \hat{a}_\alpha^\dagger | \Psi_m^{N-1}\rangle \langle\Psi_m^{N-1} | \hat{a}_\alpha | \Psi_0^N\rangle = \langle\Psi_0^N | \hat{a}_\alpha^\dagger [\hat{a}_\alpha, \hat{H}] | \Psi_0^N\rangle. \quad (6)$$

In our case, $\alpha = L, R$ and $\hat{H} = \hat{V}_1 + \hat{V}_2$, in absence of the bias. We also know,

$$[\hat{a}_L, \hat{V}_1] = 2\frac{U}{2}\hat{a}_L^\dagger\hat{a}_L\hat{a}_L, \quad [\hat{a}_L, \hat{V}_2] = -J\hat{a}_R, \quad (7)$$

and similarly for the right state. Therefore,

$$I_L + I_R = \langle\Psi_0^N | \hat{V}_1 | \Psi_0^N\rangle + 2\langle\Psi_0^N | \hat{V}_2 | \Psi_0^N\rangle. \quad (8)$$

Then the Koltum sum-rule is written as

$$\langle\Psi_0^N | \hat{H} | \Psi_0^N\rangle = \frac{1}{2}\langle\Psi_0^N | \hat{V}_1 | \Psi_0^N\rangle + \frac{1}{2}\int_{-\infty}^{\mu^-} dE E [S_h(L, L, E) + S_h(R, R, E)]. \quad (9)$$

III. RESULTS

We start by considering simplified scenarios to understand the role of the different terms. The number of particles will be always 50, unless noted otherwise.

A. Limiting cases

As shown in the Table 1, there are only three possible limiting cases.

1. Non-interacting case

In this situation, $U = 0$, and the only contribution to the energy is due to the tunnelling effect. The bias, taken much smaller than J , is irrelevant in this situation.

Case	Tunnelling	Attractive	Repulsive
Parameters	$J \neq 0$ $U = 0$	$J = 0$ $U < 0$	$J = 0$ $U > 0$
Ground State	Coherent State	Fock State	Fock State
	$ +\rangle^{\otimes N}$	$ N, 0\rangle$	$ N/2, N/2\rangle$

Table 1. The ground states of the different limiting cases with a small bias promoting the left well.

Here, the atoms are allowed to change well, but they do not interact with each other. Therefore, the problem is essentially a single particle one.

In this situation, the lowest energy corresponds to N times the energy of the sp-state $|+\rangle$, which will be fully occupied. Hence, the resulting ground state is the coherent state $|+\rangle^{\otimes N}$, which has the following expression,

$$|+\rangle^{\otimes N} = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{2}} (a_L^\dagger + a_R^\dagger) \right]^N |vac\rangle = \frac{1}{\sqrt{N!}} \frac{1}{2^{N/2}} \sum_{i=0}^N \binom{N}{i} (a_L^\dagger)^{N-i} (a_R^\dagger)^i |vac\rangle. \quad (10)$$

The coefficients, $c_i = \frac{1}{\sqrt{N!}} \frac{1}{2^{N/2}} \binom{N}{i}$, of the spectral distribution among the different Fock states correspond to a binomial distribution centered around the state $|N/2\rangle$.

The absence of interaction allows for a direct interpretation of the SPSF. Removing one particle in any occupied sp-state, for instance $|R\rangle$, $|L\rangle$ or $|+\rangle$, will not affect the other $N-1$ particles, which will remain in the ground state. Therefore, the hole SPSF for these sp-states will have only one strength different from zero, corresponding to the ground state of $N-1$ particles. For the hole SPSF of the state $|-\rangle$, the situation is different. Actually, as there are no particles in this sp-state, it is impossible to take one out and, then, $S_h(L, L; E) = 0$.

For the particle spectral function the situation is different. Notice that we can express $|R\rangle = (|+\rangle - |-\rangle)/\sqrt{2}$ and, therefore, adding a particle in the sp-state $|R\rangle$ will have half of the contribution on $|+\rangle$ and the other half on $|-\rangle$. Then, the particle SPSF will have two contributions different from zero. One from the ground state of $N+1$ particle with all the particles in the sp-state $|+\rangle$, and a tiny contribution from the first excited state, described by $|+\rangle^{\otimes N} \otimes |-\rangle$. It is easy to see that adding a particle in the sp-state $|+\rangle$ will take the system only to the ground state of $N+1$ particles, and a particle in $|-\rangle$ only to the first excited state.

2. Attractive case with no tunnelling

This case corresponds to a system of bosons that are not allowed to change wells but interact attractively with the rest of bosons of the same well. To minimize the energy, the atoms like to stay in the same well. In principle the two wells would be equally preferred, however, the

presence of the bias promotes the left well. Therefore, the ground state of the system of N particles is $|N, 0\rangle$.

This situation is completely analogous to the non-interacting case, changing $L \leftrightarrow +$ and $R \leftrightarrow -$. When $J = 0$, there was a condensate in the sp-state $|+\rangle$ and now it is in $|L\rangle$. It is easy to see that the hole part of the SPSF- $|R\rangle$ will be zero, because it is impossible to take one particle in $|R\rangle$ out of the Fock state $|N, 0\rangle$. The particle part will have only one contribution to the state $|N, 1\rangle$ which, in absence of the bias, has the same energy of $|N, 0\rangle$. That is because one particle cannot interact with itself, so it cannot contribute to the energy. On the contrary, the hole and the particle part of the SPSF- $|L\rangle$ will have only one contribution corresponding to the ground state of $N-1$ and $N+1$ respectively.

It is interesting to note, and easy to prove, that for any Fock state the SPSF of the two superposition states, $|+\rangle$ and $|-\rangle$ will be identical.

3. Repulsive case with no tunnelling

In this setting we only change the sign of U , making the interaction repulsive. Then, the system will try to form less couples as possible, resulting in another Fock state: $|N/2\rangle$. If the system has an odd number of particles, the ground state will be two-fold degenerated: $|(N+1)/2\rangle$ and $|(N-1)/2\rangle$ in absence of the bias, which has no effect.

If the number of particle is even, the hole spectral functions for R , L , $+$ and $-$ sp-states, will be identical and will have all its strength in the ground state. The same will happen for the particle spectral functions. Nevertheless, if the system have an odd number of particles it will have contributions to the first excited state when adding (removing) a particle in the well with more (less) occupation.

B. Realistic cases

Now we are ready to study the combined effects of tunnelling and interaction. The relevant parameter of the system is now $\Lambda = NU/J$.

1. Repulsive case ($\Lambda > 0$)

The effect of the repulsive interaction on the coherent state $|+\rangle^{\otimes N}$ ($\Lambda = 0$) results in a gradual transition to the Fock state $|N/2\rangle$. This transition is well-behaved, monotonous and has no singular points.

In both limits the average occupation of the right and the left well is $N/2$, and also between these two extremes. That means that this occupation is not a good witness to characterize the transition. What does change is the average occupation of the superposition states, defined

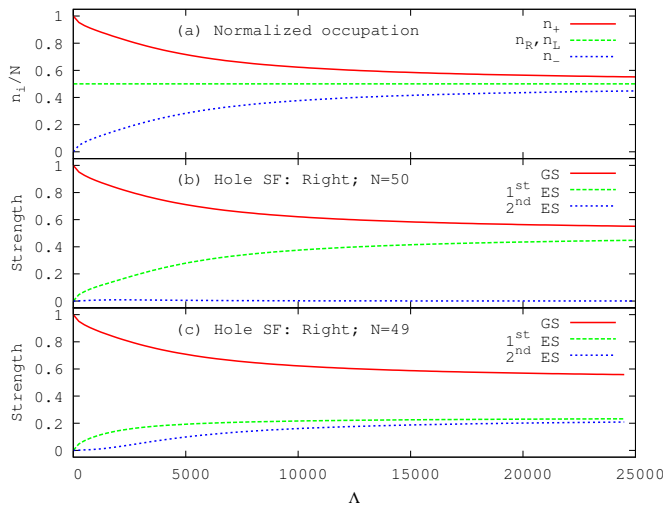


FIG. 2. Occupation and right hole spectral function for $\Lambda > 0$ (a) Occupation number of the four states considered along Λ . (b) Normalized right hole spectral strengths for the system with 50 particles. (c) Normalized right hole spectral strengths for a system of 49 particles

as $n_+ = \langle \hat{n}_+ \rangle = \langle \phi | \hat{a}_+^\dagger \hat{a}_+ | \phi \rangle$, where \hat{a}_+ is the annihilation Bose operator of the state $|+\rangle$, $\hat{a}_+ \equiv (\hat{a}_L + \hat{a}_R) / \sqrt{2}$. Similarly for n_- . Initially (by initially we refer to $\Lambda = 0$, it does not mean an evolution in time), $n_+ = N$ and $n_- = 0$, and in the final limit, they are $n_+ = n_- = N/2$, as can be seen in Fig. 2(a), where the occupations have been normalized to 1. Then, we can observe the transition by measuring these occupations.

Experimentally, however, we assume it is easier to deal with observables referred to $|R\rangle$ and $|L\rangle$, which are spatially separated. In Fig. 2(b) we have normalized to 1 the strengths of the hole SPSF- $|R\rangle$ (the system has left-right symmetry). It can be seen that the contribution of the ground state behaves as n_+ , and the strength of the first excited as n_- , showing a correlation between them. In the limit $\Lambda \rightarrow \infty$, the ground state of the system of $N - 1$ particle will be two-fold degenerated ($|25, 24\rangle$ and $|24, 25\rangle$ for an initial system of $N = 50$), if we do not take into account the little energy difference introduced by the bias. Hence, in this limit the two contributions will be located at the same energy.

This setup depends strongly on the parity of the number of particles as can be seen in Fig. 2(b-c). In the last figure, where the number of particles is odd, there is another strength caused by the second excited state. If the initial system has 49 particles, when $\Lambda \rightarrow \infty$, the system of $N-1$ particles will have a ground state: $|24, 24\rangle$ and a two-fold degenerate first excited state: $|23, 25\rangle$ and $|25, 23\rangle$. Therefore, the two strengths shown in the bottom panel corresponding to the first and second excited states, will be located at the same energy in this limit. Notice that the ground state is non-degenerate.

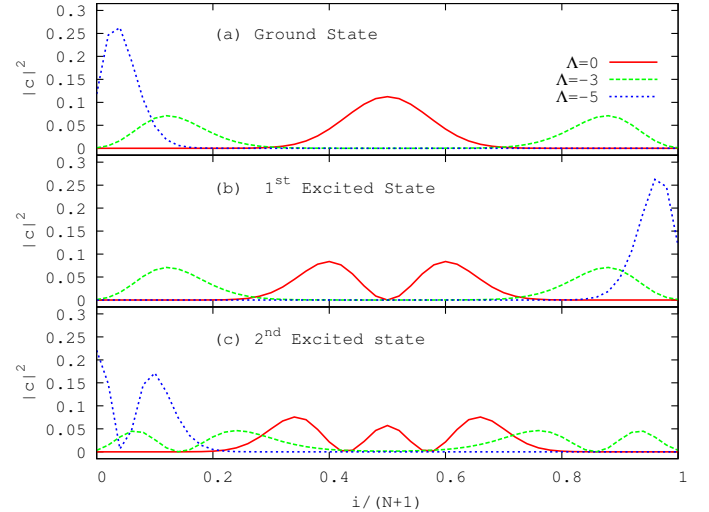


FIG. 3. States of the system when $\Lambda < 0$. (a) Ground state, (b) first excited state, and (c) second excited state.

2. Attractive case ($\Lambda < 0$)

The more interesting physics occurs in this situation, where the tunnelling competes with the attractive interaction. The system will go from a coherent state to a Fock state passing through a cat-like state, when increasing the absolute value of Λ .

First, in Fig. 3 we depict the coefficients of the three lowest energy states of the system for different values of Λ . The coefficients of the ground state correspond to a binomial distribution at first and it increases its width until it becomes a cat state (around $\Lambda = -2.2$) where the system is in a superposition of states having a macroscopic excess of particles in each of the wells. If $|\Lambda|$ keeps growing, the system 'collapses' and only a macroscopic excess in the left well survives, until it becomes, in the limit $\Lambda \rightarrow -\infty$, the Fock state $|N\rangle$.

The different types of ground states have a direct reflection on the spectral functions of the system. Looking at Fig. 4.(a-b), both spectral functions have the same behaviour until the cat-like state is lost. First the spectral functions have almost all its strength in the ground state of $N + 1$ particles. Then, around $\Lambda = 2$, this contribution starts to decrease while the corresponding to the first excited state starts to grow. This change is related to a dramatic increase of the width of the distribution of $|c_i|^2$. Then, there is an inflexion point, which is related to the emergence of the cat-like state. While this state is still the ground state of the system, both spectral functions are identical.

However, there is a point when the bias starts to contribute significantly and starts to promote the left well. Hence, the left-right symmetry is broken and the cat-like state begins to have a excess of particles in the left side. Then the first excited state is the symmetric one, with this excess on the right well. That explains why in the

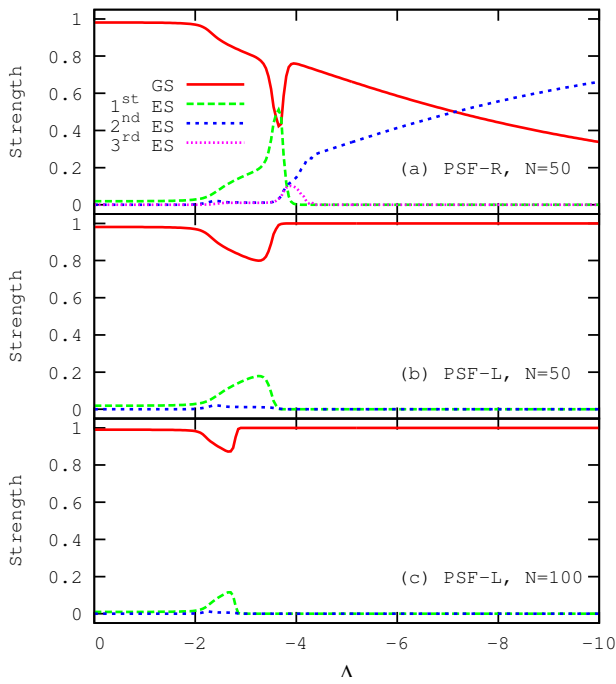


FIG. 4. Particle Spectral Functions for the attractive case. (a) Particle spectral function for the right state and $N = 50$. (b) Particle spectral function for the left state and $N = 50$. (c) Particle spectral function for the left state and $N = 100$.

particle SPSF- $|L\rangle$, the contribution of the first excited vanishes, because adding a particle in the left side promotes the system to the ground state of $N + 1$ particles, which contains also an excess of particles in the left well. On the contrary, adding a particle in the right well has a big contribution on the first excited state, where the excess is in the right side. This contribution manages to overcome the ground one until the system ‘collapses’.

After the bias makes the system go to the left well, the particle SPSF- $|L\rangle$, has only one strength corresponding to the ground state. For the particle SPSF- $|R\rangle$ (see upper panel of Fig. 4, the first excited state strength vanishes, while the contribution to the second and even the third excited states shows up. This last one only during a short range of Λ , but the corresponding to the second

one keeps growing until overcomes the ground one. As seen in the previous section, this function in the limit $\Lambda \rightarrow -\infty$ has all its strength in the first excited (second if the bias is considered), which is $|N, 1\rangle$. In absence of the bias, the ground state is two-fold degenerate between $|N, 0\rangle$ and $|0, N\rangle$, which are the limit of the ground and first excited states in this situation. Hence, the second excited state in this limit corresponds to the first excited in the previous section, where $J = 0$.

C. N Dependence

It has been already seen that the number of particles, specifically its parity, has a strong influence on the behaviour of the system. But it is interesting to note the influence of the absolute number of particles, while maintaining Λ constant.

In Fig. 4(b-c) the effect of this rise in N can be clearly seen. The effect tends to minimize the strength of the deviations from the ground state. It also causes the decrease of the (absolute) value of Λ at which the cat-like state and the collapse occur.

If the number of particles is sufficiently increased, only the contribution to the ground state will survive.

IV. SUMMARY AND CONCLUSIONS

We have explored the use of spectral functions to characterize the many-body correlators present on the ground state of a two-side Bose-Hubbard model.

The behaviour of the SPSF reveals the presence of quantum correlations in the ground state of a system and can be used together with the occupations of the natural orbits to determine if the state is in a mean field or a correlated state. We have tested the accuracy of our results by analysing the sum rules of the spectral functions.

V. ACKNOWLEDGEMENTS

Special thanks have to be rewarded to Bruno Julià Díaz and Artur Polls, who have been of a huge help during the realization of this work, due to the discussions and the orientation provided.

[1] M. Albiez, R. Gati, J. Fölling, S. Hunsmann, M. Cristiani, and M. K. Oberthaler, Phys. Rev. Lett. **95**, 010402 (2005).
 [2] J. Esteve, C. Gross, A. Weller, S. Giovanazzi, and M. K. Oberthaler, Nature (London) **455**, 1216 (2008).
 [3] C. Gross, T. Zibold, E. Nicklas, J. Estève, and M. K. Oberthaler, Nature (London) **464**, 1165 (2010).
 [4] T. Berrada, S. van Frank, R. Bücke, T. Schumm, J.-F. Schaff and J. Schmiedmayer, Nat. Commun., **4**, 2077,

(2013).
 [5] G. Mazzarella and L. Dell’Anna Eur. Phys. J. Special Topics **217**, 197-205 (2013).
 [6] B. Julià-Díaz, D. Dagnino, M. Lewenstein, J. Martorell, A. Polls, Phys. Rev. A **81**, 023615 (2010).
 [7] B. Julià-Díaz, T. Zibold, M. K. Oberthaler, M. Mele-Messeguer, J. Martorell, A. Polls, Phys. Rev. A **86**, 023615 (2012).